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Improvement of One-dimensional Gradient Shimming Method in Nuclear Magnetic Resonance Experiments

*Ce Xiao, Congbo Cai, Zhiwei Chen *, Zhong Chen*
Departments of Physics and Communications Engineering, Fujian Engineering Research Center for Solid-State Lighting, Xiamen University, Xiamen 361005, China
E-mail：　chenzhiwei@xmu.edu.cn

Abstract

Nuclear magnetic resonance (NMR) plays an important role in the fields of physics, chemistry, biology and medicine. The homogeneity of the magnetic field is very significant for NMR experiment. Based on the principle of field mapping, gradient shimming is an efficient method to achieve a homogeneous magnetic field. Reflecting accurately the spatial magnetic field distribution produced by every shim coil, gradient shimming can optimize the homogeneity efficiently and quickly. In this paper, one-dimensional gradient shimming method was studied, and the corresponding computational process was improved. Experiments were done on the NMR spectrometer, and the results show that the improved algorithm operates more efficiently and still works in a great inhomogeneous magnetic field.

1. Introduction

As a great tool for study in the fields of physics, chemistry, biology and medicine, the nuclear magnetic resonance (NMR) exhibits strong vitality and broad application prospect [1,2]. In the NMR experiment, as an important target, the homogeneity of magnetic field offers the effective assurance to the correct experimental result of NMR, which decides the realization of every characteristic of the spectrum and some pulse sequences relying highly on the homogeneous magnetic field [3]. Therefore, the method to optimize homogeneous magnetic field has been improved constantly since the invention of the NMR [4-6]. The methods include Active Shimming and Passive Shimming [7].

In the Active Shimming method, the static magnetic field B can be expressed [4] as

$$\begin{aligned} B = {} & A_1^0 + 2A_2^0 Z + 3A_2^1 X + 3B_2^1 Y + 3A_3^0(2Z^2 - X^2 - Y^2)/2 \\ & +12A_3^1 ZX + 12B_3^1 ZY + 15A_3^2(X^2 - Y^2) + 15B_3^2(2XY) \\ & +A_4^0 Z[8Z^2 - 15(X^2 + Y^2)]/2 + 15A_4^1 X(4Z^2 - X^2 - Y^2)/2 \\ & +15B_4^1 Y(4Z^2 - X^2 - Y^2)/2 + 90A_4^2 Z(X^2 - Y^2) + 90B_4^2 Z(2XY) \\ & +105A_4^3 X(X^2 - 3Y^2) + 105B_4^3 Y(3X^2 - Y^2) + \dots \end{aligned} \quad (1)$$

In order to compensate for the inhomogeneity of magnetic field, the shim coils can be designed to produce the magnetic field expressed by Eq. (1). This method was realized by adjusting the electric current values of these shim coils to optimize the homogeneity of magnetic field, so it is called Active Shimming method.

For the conventional methods of active shimming, the manual shim is troublesome and time-consuming, and requires abundant and skilled experience for the user. The automatic shim of computerized iterant search has saved time and manpower of the manual shim, but its results are limited and cannot reach a very good homogeneity. Compared with the above methods, using the spatial distribution of the magnetic field produced by shim coils to cancel the inhomogeneity of the magnetic field, gradient shimming optimizes the homogeneous magnetic field more accurately and quickly [5,6]. In the usual NMR experiments with the same background, the inhomogeneous magnetic field is mainly along the z direction caused by different samples. Besides, spinning the sample in the transverse plane of magnet can partly reduces the static magnetic field inhomogeneity except a one-dimensional problem in the z direction. In this case, we can optimize the homogeneity rapidly and efficiently via one-dimensional gradient shimming. During the process of developing NMR spectrometer, it is necessary for us to carry on the research to realize one-dimensional gradient shimming.

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2. Principle of gradient shimming

Based on the principle of magnetic resonance imaging [8], gradient shimming reflects the spatial distribution of the magnetic field by every shim coil. In order to reflect the spatial magnetic distributions of the z direction shim coils, the peak of the acquired spectrum is expanded due to a z gradient applied at the moment of sampling, as can be used to signify the distribution of magnetic field in the z direction of the sample. So we can adopt the gradient echo pulse sequence (Fig. 1) or other pulse sequences [9] with the same condition.

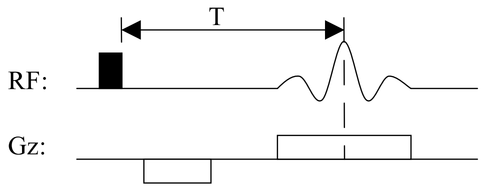

Figure 1. The gradient echo pulse sequence

In order to achieve the purpose of optimizing homogeneity, gradient shimming uses the FID data to calculate the spatial distribution of the magnetic field induced by shim coils, then the distribution of the inhomogeneous magnetic field was matched by the fitting of these effects, and the purpose of optimizing homogeneity was achieved.. In the one-dimensional gradient shimming, by analyzing many groups of FID data, we can calculate the phase difference of the peaks in two experimental spectrums and then produce shim map, the desired shim field distribution function per unit shim current. In the shimming experiment, using the field maps of shim coils to match the distribution of the inhomogeneous magnetic field, we can find out the correct shim values for homogeneous magnetic field and set them to the shim coils. Repeating the above procedure for 3-5 times, we can weaken the practical limitations, such as measurement and S/N of the profiles, and the homogeneity can be achieved within one minute.

3. Field mapping of the shim coils

The gradient echo sequence is used, and Eq. (2) gives the relationship between the phase $\varphi(z,T)$ and the magnetic field B_i(z) in the z direction.

$$\varphi(z,T) = \Omega_i(z)T + \varphi_0(z) = -\gamma B_i(z)T + \varphi_0(z) \quad (2)$$

After two continuous samplings with the different values of the time T between the pulse and the data acquisition period (Fig. 1), the unknown background constant $\varphi_0(z)$ is canceled, and then Eq. (3) can be carried out to calculate the magnetic field B_i(z) in the z direction. The deviation of the static field from its nominal value B_0 can be expressed as a function of z.

$$B_i(z) = -[\varphi(z,T1) - \varphi(z,T2)]/[\gamma(T1 - T2)] \quad (3)$$

Corresponding to the area of the peak of the spectrum received after sampling, the distribution of magnetic field in the z direction can be calculated by Eq. (3). In order to calculate the spatial distribution of the fields generated by the individual z direction shim coil, a procedure for shim mapping is designed with different B_i(z). With B_i(z) under a defined shim coil current increment I_i and the initial B_0(z), the shim map S_i(z) of shim coil *Zi* can be calculated as

$$S_i(z) = (B_i(z) - B_0(z)) / I_i \quad (4)$$

Each of the shim coils will produce its shim map through the procedure, and the total results are the shim maps that we need.

Phase wrap is a problem that needed to be treated carefully. While calculating the phase, the value of phase will have been wrapped into the range [-π, π] or [0, 2π]. If the data gives phase differences that are small enough to fall into this range, the measured phase can be used directly. Unfortunately, the phase difference for the field mapping is often too large to be inside the range. To recover the true phase, we must restore the missing multiples of 2kπ. The phase wrap can destroy the continuity of the phase data. By adopting the improved phase unwrap technology [10], we can solve this problem effectively, and can recover the continuity of the data under some distorted situation.

4. Improvement of shimming algorithms

The distribution of the inhomogeneous magnetic field along the z direction can be got with the method of field mapping. In the shimming experiment, the field map of every shim coil must be provided to fit the distribution of the inhomogeneous magnetic field, and thus the appropriate electric current value for every shim coil can be calculated. By setting these corresponding electric current values to the shim coils, a simple procedure of gradient shimming can be performed.

The variance of the distribution data of inhomogeneous magnetic field was used as the criterion to judge the fitting result of the field maps. The goal of shimming is to get a more homogeneous magnetic field. Therefore, the variance of the distribution data of the inhomogeneous magnetic field shows the homogeneity, and the smaller variance represents the more homogeneous magnetic field after shimming.

Supposing that the variance value can be zero, the fitting calculation process can be treated as solving a linear equations group, and thus some basic methods can be applied, such as the Gauss elimination approach. These methods are currently applied mostly in the spectrometers. However, because of the limit of precision for the shim coil's electric current value, the result calculated by the above methods would have some error, which reduces the calculation accuracy. Therefore, the shimming effects may be limited. Furthermore, this method cannot work smoothly in great inhomogeneous magnetic field because of the rough data of field mapping.

In order to solve the problem and get more exact values of shim coils, we proposed an improved calculation algorithm. According to the principle of the greedy algorithm [11], we designed a new fitting algorithm with the strategy of repeated cycles of the high and low rank shim coils. A search algorithm with fast convergence was adopted. The variance of one-dimensional data, which represents new distribution of magnetic field in each calculation step, was used as the calculation criterion. The optimum value of coil electric current corresponded to the minimum of variance value. From the low rank to high rank and then back to the low rank coils, circulating repeatedly several times, the error can be reduced to a low level that reach the demand. Increasing the influence of the low rank shim coils, the above sequence of shim coils can be used to reduce the inhomogeneity faster and more rationally. The number of repeated calculation was limited and decided by the necessary error claim. The process of calculation will be completed within one second, and the shim maps can be utilized to fit the distribution data of inhomogeneous magnetic field more effectively and rapidly, and the homogeneous magnetic field can be got.

5. Experimental results and discussion

The improved algorithm was programmed in the Java development kit 1.60. The corresponding experiments were done in Varian System 500 MHz Spectrometer with ID probe and the solute sample of 1% H_2O and 99% D_2O. The shim maps were prepared under a homogeneous magnetic field before the verifiable experiment. After the sampling procedures repeating for 12 times with the same gradient echo pulse sequence, the shim maps of Z1 to Z5 shim coils were calculated with the FID data. The shim maps were shown in Fig. 2. In the experiment, we set the electric current values of Z1 to Z5 shimming coils to

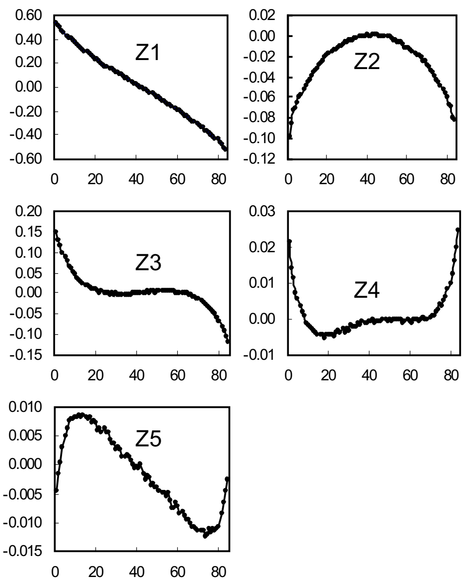

Figure 2. Shim maps of Z1 to Z5 shim coils

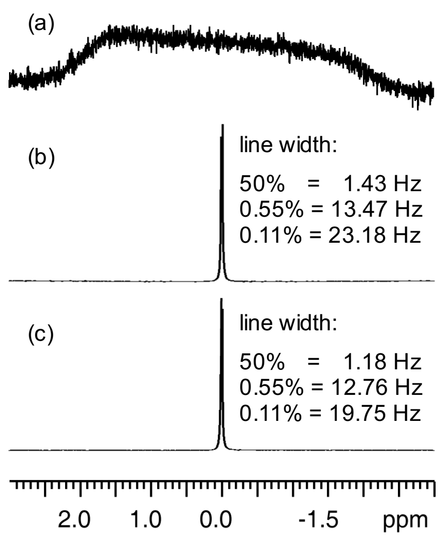

Figure 3. (a) The nonspinning ^{1}H spectrum with zero values of Z1 to Z5 coils and 152.51 Hz of the 50% line width; (b) the nonspinning ^{1}H spectrum after Varian's 1D gradient shimming with 3 iterations and 1.43 Hz of the 50% line width; (c) the nonspinning ^{1}H spectrum after new 1D gradient shimming with 3 iterations and 1.18 Hz of the 50% line width.

be zero as the inhomogeneous magnetic field, and the 50% line width was 152.51 Hz (Fig. 3(a)). After gradient shimming in Varian software with 3 iterations from the initial field, the 50% line width was reduced to 1.43 Hz (Fig. 3(b)). However, the 50% line width can be reduced to about 1.18 Hz by our improved algorithm under the same experimental condition (Fig. 3(c)). The process of one-dimensional gradient shimming was done in one minute. According to the experimental results, the improved algorithm of one-dimensional gradient shimming works more rapidly and efficiently.

In another experiment with all shim coils set to zero, the gradient shimming method in Varian software was failed. But the new algorithm still worked, and the 50% line width was reduced from 148.2 Hz to 12.0 Hz. A further study in optimizing the gradient shimming algorithm under the huge inhomogeneity will be carried on.

If the sampling data was distorted in the field mapping, the calculated results will be not reliable, so re-sampling is needed. The inhomogeneous magnetic field itself will also influence the accuracy of field mapping. Therefore, the correct shim maps should be prepared under the homogeneous magnetic field to assure a successful gradient shimming in ordinary experiments.

Because of the influence between low and high rank shim coils and other practical limitations, gradient shimming usually cannot reach the optimum results once. 3 to 5 times iterations of gradient shimming can solve this problem, and the procedure will adjust necessary repeated times automatically according to the changing values of shim coils. If the iteration is still needed after changing the values of shim coils greatly for many times, it means that the field maps are incorrect, and you will be asked automatically to load a new and correct shim map instead of the current one.

6. Conclusion

As shown in the experimental results, the designed one-dimensional gradient shimming method is proved to be correct and effective. The improved calculation algorithm of shimming field helps a lot for calculating the accurate electric current value of shim coils. As an important part of the development of NMR spectrometer, one-dimensional gradient shimming decides the performance of the shimming system, and can act as a solid basis for achieving three-dimensional gradient shimming in the further.

Acknowledgments

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